NEWS IPC8

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FILE 'HOME' ENTERED AT 15:50:32 ON 07 JUN 2007

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.42 0.42

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 15:51:34 ON 07 JUN 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 JUN 2007 HIGHEST RN 936692-95-4 DICTIONARY FILE UPDATES: 6 JUN 2007 HIGHEST RN 936692-95-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\161.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full FULL SEARCH INITIATED 15:52:17 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 20 TO ITERATE

100.0% PROCESSED 20 ITERATIONS SEARCH TIME: 00.00.01

0 ANSWERS

=> s l1 full

FULL SEARCH INITIATED 15:53:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 20 TO ITERATE

100.0% PROCESSED

20 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L3

0 SEA SSS FUL L1

=> file reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY

SESSION

346.00

346.42

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 15:55:27 ON 07 JUN 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 JUN 2007 HIGHEST RN 936692-95-4 DICTIONARY FILE UPDATES: 6 JUN 2007 HIGHEST RN 936692-95-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

Uploading C:\Program Files\Stnexp\Queries\161a.str

L4 STRUCTURE UPLOADED

=> d;4

L4 HAS NO ANSWERS

L4 STR

Structure attributes must be viewed using STN Express query preparation.

4 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> s l4 sss full

FULL SEARCH INITIATED 15:56:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 29 TO ITERATE

100.0% PROCESSED

29 ITERATIONS

27 ANSWERS

SEARCH TIME: 00.00.01

L5

27 SEA SSS FUL L4

=> d 15 1-27

L5 ANSWER 1 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 892396-78-0 REGISTRY

ED Entered STN: 13 Jul 2006

CN Benzenepropanoic acid, $\alpha-[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (-)-, compd. with <math>(\alpha S)-\alpha-ethyl-2-naphthalenemethanamine (1:1) (9CI) (CA INDEX NAME)$

FS STEREOSEARCH

MF C26 H28 O7 S2 . C13 H15 N

SR C

LC STN Files: CA, CAPLUS

CM 1

CRN 549494-39-5 CMF C26 H28 O7 S2

Absolute stereochemistry. Rotation (-).

CM 2

CRN 254437-90-6 CMF C13 H15 N

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 2 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 892396-76-8 REGISTRY

ED Entered STN: 13 Jul 2006

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (-)-, compd. with (α R)- α -ethyl-1-naphthalenemethanamine (1:1) (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H28 O7 S2 . C13 H15 N

SR CA

LC STN Files: CA, CAPLUS

CM 1

CRN 549494-39-5 CMF C26 H28 O7 S2

Absolute stereochemistry. Rotation (-).

CM 2

CRN 22038-83-1 CMF C13 H15 N

Absolute stereochemistry.

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 3 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 892396-73-5 REGISTRY
- ED Entered STN: 13 Jul 2006
- CN Cinchonan-9-ol, $(8\alpha, 9R)$ -, mono[(-)- α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]benze nepropanoate] (salt) (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C26 H28 O7 S2 . C19 H22 N2 O
- SR CA
- LC STN Files: CA, CAPLUS

CM 1

CRN 549494-39-5

Absolute stereochemistry. Rotation (-).

CM 2

CRN 485-71-2 CMF C19 H22 N2 O

Absolute stereochemistry. Rotation (-).

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 4 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 891182-81-3 REGISTRY

ED Entered STN: 10 Jul 2006

CN Benzenepropanoic acid, $\alpha-[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (-)-, compd. with 2-methyl-2-propanamine (1:1) (9CI) (CA INDEX NAME)$

FS STEREOSEARCH

MF C26 H28 O7 S2 . C4 H11 N

SR CA

LC STN Files: CA, CAPLUS, CASREACT

CM 1

CRN 549494-39-5 CMF C26 H28 O7 S2

Absolute stereochemistry. Rotation (-).

CM 2

CRN 75-64-9 CMF C4 H11 N

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 5 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 891182-74-4 REGISTRY

ED Entered STN: 10 Jul 2006

CN Benzenepropanoic acid, $4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-\alpha-[(2-phenylethyl)thio]-, (<math>\alpha$ S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H28 O6 S2

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 6 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 840494-28-2 REGISTRY
- ED Entered STN: 02 Mar 2005
- CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, ion(1-) (9CI) (CA INDEX NAME)
- MF C26 H27 O7 S2
- CI COM
- SR CA

$$\begin{array}{c|c} O & CO_2 \\ \hline \\ O & CH_2 - CH_2 \\ \hline \end{array}$$

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L5 ANSWER 7 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
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RN 817642-79-8 REGISTRY

ED Entered STN: 21 Jan 2005

CN Benzenepropanoic acid, $\alpha-[[2-[4-(1,1-dimethylethoxy)phenyl]]$ thi o]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME) OTHER NAMES:

CN 2-[[2-(4-tert-Butoxyphenyl)ethyl]sulfanyl]-3-[4-[2-[4-[(methanesulfonyl)oxy]phenoxy]ethyl]phenyl]propionic acid

MF C30 H36 O7 S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PAGE 1-A

PAGE 1-B

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 8 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817642-78-7 REGISTRY

ED Entered STN: 21 Jan 2005

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]-2-(phenylmethyl)phenoxy]ethyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 3-[4-[2-[2-benzyl-4-[(methanesulfonyl)oxy]phenoxy]ethyl]phenyl]-2-[[2-(4-hydroxyphenyl)ethyl]sulfanyl]propionic acid

MF C33 H34 O7 S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PAGE 1-A

__ OH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 9 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 817642-76-5 REGISTRY
- ED Entered STN: 21 Jan 2005
- CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]sulfonyl]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

- CN 2-[[2-(4-Hydroxyphenyl)ethyl]sulfonyl]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid
- MF C26 H28 O9 S2
- SR CA
- LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PAGE 1-B

__ OH

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 10 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN:
- RN 817642-73-2 REGISTRY
- ED Entered STN: 21 Jan 2005
- CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]sulfinyl]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME) OTHER NAMES:
- CN 2-[[2-(4-Hydroxyphenyl)ethyl]sulfinyl]-3-[4-[2-[4-
 - [(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid
- MF C26 H28 O8 S2
- SR CA
- LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PAGE 1-A

PAGE 1-B

__ OH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

· 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 11 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817642-72-1 REGISTRY

ED Entered STN: 21 Jan 2005

CN Benzenepropanoic acid, α -[[2-(3-methoxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 2-[[2-(3-Methoxyphenyl)ethyl]thio]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid

MF C27 H30 O7 S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PAGE 1-A

$$\begin{array}{c} \circ \\ \text{Me-s-o} \\ \circ \\ \circ \\ \text{O} \end{array}$$

PAGE 1-B

_ oMe

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 12 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 817642-71-0 REGISTRY
- ED Entered STN: 21 Jan 2005
- CN Benzenepropanoic acid, α -[[2-(2-fluorophenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME) OTHER NAMES:

CN 2-[[2-(2-Fluorophenyl)ethyl]thio]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid

MF C26 H27 F O6 S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

$$\begin{array}{c} O \\ Me-S-O \\ O \\ O \\ O \\ CH_2-CH_2 \\ \end{array} \begin{array}{c} CO_2H \\ F \\ CH_2-CH_2-CH_2 \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 13 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817642-69-6 REGISTRY

ED Entered STN: 21 Jan 2005

CN Benzenepropanoic acid, α -[[2-[4-(dimethylamino)phenyl]ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME) OTHER NAMES:

CN 2-[[2-[4-(Dimethylamino)phenyl]ethyl]thio]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid

MF C28 H33 N O6 S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PAGE 1-A

$$\begin{array}{c} \circ \\ \text{Me-s-o} \\ \circ \\ \circ \\ \text{O} \end{array} \begin{array}{c} \text{CO}_2\text{H} \\ \text{CH}_2\text{-CH-s-CH}_2\text{-CH}_2 \end{array}$$

PAGE 1-B

 \sim NMe₂

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- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 14 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 817209-96-4 REGISTRY
- ED Entered STN: 20 Jan 2005
- CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]benze nepropanoic acid (1:1) (9CI) (CA INDEX NAME)
- MF C26 H27 O7 S2 . C5 H14 N O
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 840494-28-2 CMF C26 H27 O7 S2

PAGE 1-A

$$\begin{array}{c} \begin{array}{c} \\ \text{Me-s-o} \\ \\ \text{O} \end{array} \\ \begin{array}{c} \text{CO}_2^- \\ \\ \text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_2 \end{array}$$

PAGE 1-B

__ OH

CM 2

CRN 62-49-7 CMF C5 H14 N O

 $Me_3+N-CH_2-CH_2-OH$

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 15 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817209-95-3 REGISTRY

ED Entered STN: 20 Jan 2005

CN Benzenepropanoic acid, $\alpha-[[2-(4-\text{hydroxyphenyl})\text{ethyl}]\text{thio}]-4-[2-[4-[(methylsulfonyl)\text{oxy}]\text{phenoxy}]\text{ethyl}]-, compd. with tricyclo[3.3.1.13,7]decan-1-amine (1:1) (9CI) (CA INDEX NAME)$

MF C26 H28 O7 S2 . C10 H17 N

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

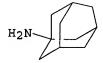
CRN 549494-28-2 CMF C26 H28 O7 S2

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CM 2

CRN 768-94-5 CMF C10 H17 N



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 16 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817209-93-1 REGISTRY

ED Entered STN: 20 Jan 2005

CN L-Lysine, mono [α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]benzenepropanoate] (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H28 O7 S2 . C6 H14 N2 O2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

PAGE 1-A

$$\begin{array}{c} \circ \\ \parallel \\ \text{Me-s-o} \\ \parallel \\ \circ \\ \text{O} \\ \end{array} \begin{array}{c} \text{CO}_2\text{H} \\ \parallel \\ \text{CH}_2-\text{CH-s-CH}_2-\text{CH}_2 \end{array}$$

PAGE 1-B

__ OH

CM 2

CRN 56-87-1

CMF C6 H14 N2 O2

Absolute stereochemistry.

$$\begin{array}{c|c}
NH_2\\
NH_2\\
S
\end{array}$$
 $\begin{array}{c|c}
(CH_2) & 4
\end{array}$

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 17 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817209-92-0 REGISTRY

ED Entered STN: 20 Jan 2005

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

MF C26 H28 O7 S2 . C4 H11 N O3

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

PAGE 1-A

$$\begin{array}{c} \circ \\ \text{Me-s-o} \\ \circ \\ \circ \\ \text{O-CH}_2\text{-CH}_2 \\ \end{array} \begin{array}{c} \text{CO}_2\text{H} \\ \text{CH}_2\text{-CH-s-CH}_2\text{-CH}_2 \\ \end{array}$$

PAGE 1-B

__ OH

CM 2

CRN 77-86-1 CMF C4 H11 N O3

$$\begin{array}{c} {\rm NH_2} \\ | \\ {\rm HO-CH_2-C-CH_2-OH} \\ | \\ {\rm CH_2-OH} \end{array}$$

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 18 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817209-91-9 REGISTRY

ED Entered STN: 20 Jan 2005

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, compd. with piperazine (1:1) (9CI) (CA INDEX NAME)

MF C26 H28 O7 S2 . C4 H10 N2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

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PAGE 1-B

__ OH

CM 2

CRN 110-85-0 CMF C4 H10 N2

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 19 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817209-90-8 REGISTRY

ED Entered STN: 20 Jan 2005

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, compd. with 2-methyl-2-propanamine (1:1) (9CI) (CA INDEX NAME)

MF C26 H28 O7 S2 . C4 H11 N

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

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PAGE 1-B

CM 2

CRN 75-64-9 CMF C4 H11 N

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 20 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817181-58-1 REGISTRY

ED Entered STN: 20 Jan 2005

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (α R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H28 O7 S2

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Absolute stereochemistry. Rotation (+).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 21 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 815608-42-5 REGISTRY

ED Entered STN: 18 Jan 2005

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, sodium salt, (α S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H28 O7 S2 . x Na

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CRN (549494-39-5)

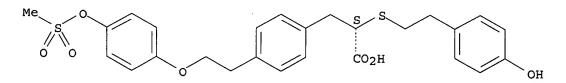
Absolute stereochemistry. Rotation (-).

●x Na

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 22 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 815608-41-4 REGISTRY
- ED Entered STN: 18 Jan 2005
- CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, potassium salt, (α S)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C26 H28 O7 S2 . x K
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL
- CRN (549494-39-5)

Absolute stereochemistry. Rotation (-).



●x K

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 23 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 549494-39-5 REGISTRY
- ED Entered STN: 17 Jul 2003
- CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (α S)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C26 H28 O7 S2
- CI COM
- SR CA
- LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 6 REFERENCES IN FILE CA (1907 TO DATE)
- 6 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 24 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 549494-32-8 REGISTRY
- ED Entered STN: 17 Jul 2003
- CN Benzenepropanoic acid, α -[[2-(4-chlorophenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (-)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C26 H27 Cl O6 S2
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 25 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 549494-29-3 REGISTRY
- ED Entered STN: 17 Jul 2003
- CN Benzenepropanoic acid, α -[[2-(4-fluorophenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)
- MF C26 H27 F O6 S2
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

PAGE 1-A

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 26 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 549494-28-2 REGISTRY

ED Entered STN: 17 Jul 2003

CN Benzenepropanoic acid, α-[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

MF C26 H28 O7 S2

CI COM

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

PAGE 1-A

PAGE 1-B

__ OH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 27 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 549494-27-1 REGISTRY

ED Entered STN: 17 Jul 2003

CN Benzenepropanoic acid, α -[[2-(4-chlorophenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

MF C26 H27 Cl O6 S2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

PAGE 1-A

PAGE 1-B

__c1

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

572.07

225.65

FULL ESTIMATED COST

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FILE 'REGISTRY' ENTERED AT 15:51:34 ON 07 JUN 2007

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L3 0 S L1 FULL

FILE 'REGISTRY' ENTERED AT 15:55:27 ON 07 JUN 2007

L4 STRUCTURE UPLOADED

L5 27 S L4 SSS FULL

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MISSING OPERATOR L5 IBIB
The search profile that was entered contains terms or

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L6 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2006:608744 CAPLUS

DOCUMENT NUMBER:

145:83117

TITLE:

Preparation of amine salts of (-)-2-((2-(4-hydroxyphenyl)ethyl)thio)-3-(4-(2-(4-

((methylsulfonyl)oxy) phenoxy)ethyl)phenyl) propanoic acid for treating lipid disorders Snape, Evan William Astrazeneca AB, Swed.; Astrazeneca UK Limited PCT Int. Appl., 24 pp. CODEN: PIXXD2 Patent English FAMILY ACC. NUM. COUNT: KIND DATE APPLICATION NO. DATE ----A1 20060622 WO 2005-GB4829 20051214 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM GB 2004-27701 A 20041217 A cinchonidine salt, an (R)-(+)-1-(1-naphthyl)ethylamine salt and a (S)-(-)-1-(2-naphthyl)ethylamine salt of the title compound (I) processes for their preparation, their use in treating clin. conditions including lipid disorders (dyslipidemias) whether or not associated with insulin resistance and other manifestations of the metabolic syndrome, and pharmaceutical compns. containing them, are described. 892396-73-5P 892396-76-8P 892396-78-0P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (preparation of amine salts of (-)-2-((2-(4-hydroxyphenyl)ethyl)thio)-3-(4-(2-(4-((methylsulfonyl)oxy) phenoxy)ethyl)phenyl) propanoic acid for treating lipid disorders) 892396-73-5 CAPLUS Cinchonan-9-ol, $(8\alpha, 9R)$ -, mono $[(-)-\alpha-[[2-(4$ hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]benze nepropanoate] (salt) (9CI) (CA INDEX NAME)

CM 1

(Uses)

IT

RN

CN

INVENTOR (S):

DOCUMENT TYPE:

SOURCE:

LANGUAGE:

PATENT ASSIGNEE(S):

PATENT INFORMATION:

PATENT NO.

PRIORITY APPLN. INFO.:

-----WO 2006064232

CRN 549494-39-5 CMF C26 H28 O7 S2

Absolute stereochemistry. Rotation (-).

CM 2

CRN 485-71-2 CMF C19 H22 N2 O Absolute stereochemistry. Rotation (-).

RN 892396-76-8 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (-)-, compd. with (αR) - α -ethyl-1-naphthalenemethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 549494-39-5 CMF C26 H28 O7 S2

Absolute stereochemistry. Rotation (-).

CM 2

CRN 22038-83-1 CMF C13 H15 N

Absolute stereochemistry.

RN 892396-78-0 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (-)-, compd. with (α S)- α -ethyl-2-naphthalenemethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 549494-39-5

Absolute stereochemistry. Rotation (-).

CM 2

CRN 254437-90-6 CMF C13 H15 N

Absolute stereochemistry.

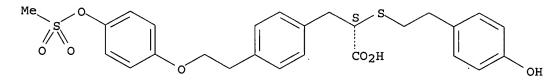
IT 549494-39-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amine salts of (-)-2-((2-(4-hydroxyphenyl)ethyl)thio)-3-(4-(2-(4-((methylsulfonyl)oxy) phenoxy)ethyl)phenyl) propanoic acid for treating lipid disorders)

RN 549494-39-5 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2006:608672 CAPLUS

DOCUMENT NUMBER:

145:61508

TITLE:

Chemoenzymic synthesis of 3-phenyl-2arylalkylthiopropionic acid derivatives

INVENTOR(S):

arylalkylthiopropionic acid derivatives Brown, David; Gilday, John Peter; Hopes, Philip

Anthony; Moseley, Jonathan David; Snape, Evan William;

Wells, Andrew

PATENT ASSIGNEE(S):

Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE: PCT Int. Appl., 52 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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	WO 2006						20060824											
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		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KN,	ΚP,	KR,	
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		MZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	
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		CF,	VE.	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,	
		WC	KZ,	MD,	DII,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,	
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Absolute stereochemistry.

IT 549494-39-5P

RL: BPN (Biosynthetic preparation); CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent) (chemoenzymic synthesis of 3-phenyl-2-arylalkylthiopropionic acid derivs.)

RN 549494-39-5 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 817181-58-1P

RL: BYP (Byproduct); PREP (Preparation)
 (chemoenzymic synthesis of 3-phenyl-2-arylalkylthiopropionic acid
 derivs.)

RN 817181-58-1 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (α R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 891182-81-3P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(chemoenzymic synthesis of 3-phenyl-2-arylalkylthiopropionic acid derivs.)

RN -891182-81-3 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (-)-, compd. with 2-methyl-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 549494-39-5 CMF C26 H28 O7 S2

Absolute stereochemistry. Rotation (-).

CM 2

CRN 75-64-9 CMF C4 H11 N

IT 549494-28-2

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent) (chemoenzymic synthesis of 3-phenyl-2-arylalkylthiopropionic acid derivs.)

RN 549494-28-2 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} O \\ Me-s-O \\ O \\ O \\ O \\ O \\ O \\ O-CH_2-CH_2 \\ \end{array} \begin{array}{c} CO_2H \\ CH_2-CH-s-CH_2-CH_2 \\ \end{array}$$

PAGE 1-B

__ OH

IT 817209-90-8P

RL: PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)

(chemoenzymic synthesis of 3-phenyl-2-arylalkylthiopropionic acid derivs.)

RN 817209-90-8 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, compd. with 2-methyl-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

PAGE 1-A

$$\begin{array}{c} \circ \\ \text{Me-s-o} \\ \circ \\ \circ \\ \text{O-CH}_2\text{-CH}_2 \\ \end{array}$$

PAGE 1-B

__ OH

CM 2

CRN 75-64-9 CMF C4 H11 N

NH₂ | H₃C-C-CH₃ | CH₃

ACCESSION NUMBER: 2004:1154663 CAPLUS DOCUMENT NUMBER: 142:93390 TITLE: Process for the preparation of racemic [(hydroxyphenyl)ethylthio]propanoic acid derivative, useful as selective PPARa modulator INVENTOR(S): Andersson, Kjell; Lindstedt-Astermark, Eva-Lotte; Sorensen, Henrik PATENT ASSIGNEE(S): Astrazeneca Ab, Swed.; Astrazeneca Uk Limited SOURCE: PCT Int. Appl., 17 pp. CODEN: PIXXD2 DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE ------------WO 2004113285 A1 20041229 WO 2004-GB2599 20040616 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR; HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG AU 2004249487 **A1** 20041229 AU 2004-249487 20040616 CA 2529252 Α1 20041229 CA 2004-2529252 20040616 EP 1638929 A1 20060329 EP 2004-736920 20040616 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR BR 2004011450 Α 20060718 BR 2004-11450 20040616 CN 1835918 Α 20060920 CN 2004-80023145 20040616 JP 2006527751 Т 20061207 JP 2006-516435 20040616 NO 2005005883 Α 20060109 NO 2005-5883 20051212 US 2006167309 A1 20060727 US 2005-561161 20051216 PRIORITY APPLN. INFO.: GB 2003-14260 A 20030619 WO 2004-GB2599 W 20040616 OTHER SOURCE(S): CASREACT 142:93390; MARPAT 142:93390 The invention provides a process for preparation of racemic [(hydroxyphenyl)ethylthio]propanoic acid derivative of formula I, useful as selective PPAR α modulator (no biol. data). The racemic title compound I was prepared via thiolation of 2-chloropropanoate derivative II by 2-[4-(benzyloxy)phenyl]ethanethiol, debenzylation, and hydrolysis. Resolution of I gave (-)-I and (+)-I. (+)-Enantiomer was used as a starting material for racemization reaction. IT549494-39-5P RL: IMF (Industrial manufacture); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation) (process for the preparation of racemic [(hydroxyphenyl)ethylthio]propanoic acid derivative useful as selective PPARa modulator) 549494-39-5 CAPLUS RNCNBenzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (\alphaS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 549494-28-2P 817181-58-1P

> RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(process for the preparation of racemic [(hydroxyphenyl)ethylthio]propanoic

acid derivative useful as selective PPARa modulator)

RN549494-28-2 CAPLUS

Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-CN[(methylsulfonyl)oxy]phenoxy]ethyl] - (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} \begin{array}{c} \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \end{array}$$

PAGE 1-B

__ OH

RN817181-58-1 CAPLUS

Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-CN [(methylsulfonyl)oxy]phenoxy]ethyl]-, (\alpha R) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

5

ACCESSION NUMBER:

2004:1154662 CAPLUS

DOCUMENT NUMBER:

142:86664

TITLE:

SOURCE:

Potassium or sodium salt of $(-)-2-\{[2-(4-$

hydroxyphenyl) ethyl] thio $\}$ -3 - [4 - (2 - $\{4$ -

[(methylsulfonyl)oxy]phenoxy}ethyl)phenyl]propanoic

acid and their use in medicine

INVENTOR(S):

Ahlqvist, Matti; Bohlin, Martin Hans

PATENT ASSIGNEE(S):

Astrazeneca AB, Swed.; Astrazeneca UK Limited

PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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                                  DATE
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     WO 2004113284
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                                  20041229
                                              WO 2004-GB2595
                                                                       20040616
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     BR 2004011515
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                                                                       20051216
PRIORITY APPLN. INFO.:
                                              GB 2003-14131
                                                                   Α
                                                                       20030618
                                              WO 2004-GB2595
                                                                   W
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AΒ
     A potassium salt or a sodium salt of (-)-2-\{[2-(4-
     hydroxyphenyl)ethyl]thio}-3-[4-(2-{4-[(methylsulfonyl)oxy]phenoxy}ethyl)ph
     enyl]propanoic acid, processes for their preparation, their use in treating
     clin. conditions including lipid disorders (dyslipidemias) whether or not
     associated with insulin resistance and other manifestations of the metabolic
     syndrome, and pharmaceutical compns. containing them.
IT
     815608-41-4P 815608-42-5P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of potassium or sodium salt of (-)-2-\{[2-(4-
        hydroxyphenyl)ethyl]thio}-3-[4-(2-{4-[(methylsulfonyl)oxy]phenoxy}ethyl
        )phenyl]propanoic acid for therapeutic use)
RN
     815608-41-4 CAPLUS
     Benzenepropanoic acid, \alpha-[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-
CN
```

Absolute stereochemistry. Rotation (-).

[(methylsulfonyl)oxy]phenoxy]ethyl]-, potassium salt, (αS) - (9CI)

●v 16

RN 815608-42-5 CAPLUS

(CA INDEX NAME)

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, sodium salt, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

●x Na

IT 549494-39-5P

RL: PUR (Purification or recovery); PREP (Preparation)
 (preparation of potassium or sodium salt of (-)-2-{[2-(4-

hydroxyphenyl)ethyl]thio}-3-[4-(2-{4-[(methylsulfonyl)oxy]phenoxy}ethyl

)phenyl]propanoic acid for therapeutic use)

RN 549494-39-5 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 549494-28-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of potassium or sodium salt of (-)-2-{[2-(4-hydroxyphenyl)ethyl]thio}-3-[4-(2-{4-[(methylsulfonyl)oxy]phenoxy}ethyl)phenyl)propanoic acid for therapeutic use)

RN 549494-28-2 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

__ OH

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2004:1154661 CAPLUS

DOCUMENT NUMBER:

142:93515

TITLE:

A preparation of amine salts of

[(phenoxyethyl)phenyl]propanoic acid derivative,

useful for the treatment of lipid disorders

INVENTOR (S):

Ahlqvist, Matti; Dahlstrom, Mikael Ulf Johan; Ohlsson,

Bengt; Storey, Richard Anthony; Taylor, Nigel Philip;

Woods, Rebecca

CODEN: PIXXD2

PATENT ASSIGNEE(S):

Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE:

PCT Int. Appl., 43 pp.

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

		ENT								APPLICATION NO.										
						A1 20041229										0040	 616			
		W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,		
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,		
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,		
			LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,		
												SC,								
												UZ,								
		RW:	BW,	GH,	GM,	KΕ,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,		
			ΑZ,	BY,	KG,	KZ,	MD,	RU,	ТJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK.		
			EE,	ES,	FI,	FR,	GB,	GR;	ΗU,	ΙE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,		
			SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE.		
				TD,											•	·	•	-,		
	ΑU	AU 2004249483					A1 20041229				AU 2004-249483						20040616			
		A 2529544						2004	1229	CA 2004-2529544						20040616				
	ĒΡ	, 1638930					A1 20060329				EP 2004-736922						20040616			
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,		
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		2004	0115	80		Α		2006	8080		BR 2	004-	1158	0		20	0040	616		
	CN	1835	919			Α		2006	0920	CN 2004-80023146						20040616				
	JP 2006527749							2006	1207	1	JP 2006-516428						20040616			
	NO 2005006006							A 20060224			NO 2005-6006						20051216			
	US	2007	0999:	28		A1		2007	0503	1	US 2005-561222						20051219			
PRIC	RITY	APP:	LN.	INFO	. :												A 20030618			
										1	WO 2	004-0	GB25	76	1	N 20	0040	616		
AB	The	inve	enti	on r	elat	es to	оа	prep	arat	ion (of t	ert-	buty:	lamiı	ne sa	alt,	pipe	erazi	ine	

salt, choline salt, tris(hydroxymethyl)methylamine salt, lysine salt, or adamantylamine salt of [(phenoxyethyl)phenyl]propanoic acid derivative of formula (-)-I, useful in the treatment of lipid disorders (no biol. data). Tert-Butylamine salt of (-)-I was prepared from (-)-I and tert-butylamine with a yield of 68% (example 1).

IT 817209-90-8P 817209-91-9P 817209-92-0P 817209-93-1P

> RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of amine salts of [(phenoxyethyl)phenyl]propanoic acid derivative

useful for the treatment of lipid disorders)

RN 817209-90-8 CAPLUS

Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-CN [(methylsulfonyl)oxy]phenoxy]ethyl]-, compd. with 2-methyl-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

PAGE 1-A

PAGE 1-B

__ OH

CM 2

CRN 75-64-9 CMF C4 H11 N

RN 817209-91-9 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, compd. with piperazine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

PAGE 1-A

$$\begin{array}{c} O \\ Me-S-O \\ O \\ O \\ O \\ O \\ O-CH_2-CH_2 \end{array} \begin{array}{c} CO_2H \\ CH_2-CH-S-CH_2-CH_2 \\ \end{array}$$

PAGE 1-B

__ OH

CM 2

CRN 110-85-0 CMF C4 H10 N2

RN 817209-92-0 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

PAGE 1-A

$$\begin{array}{c|c} O & CO_2H & CO_2H \\ \hline \\ O & O-CH_2-CH_2 & CH_2-CH_2-CH_2 \\ \hline \end{array}$$

PAGE 1-B

__ OH

CM 2

CRN 77-86-1 CMF C4 H11 N O3

$$^{\mathrm{NH_2}}_{\mathrm{HO-CH_2-C-CH_2-OH}}$$

RN 817209-93-1 CAPLUS

CN L-Lysine, mono [α -[{2-(4-hydroxyphenyl)ethyl]thio}-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]benzenepropanoate] (9CI) (CA INDEX NAME)

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

PAGE 1-A

__ OH

CM 2

CRN 56-87-1 CMF C6 H14 N2 O2

Absolute stereochemistry.

IT 817209-95-3P 817209-96-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

 $\label{lem:condition} \mbox{(preparation of amine salts of [(phenoxyethyl)phenyl]propanoic acid derivative}$

useful for the treatment of lipid disorders)

RN 817209-95-3 CAPLUS

CN Benzenepropanoic acid, $\alpha-[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, compd. with tricyclo[3.3.1.13,7]decan-1-amine (1:1) (9CI) (CA INDEX NAME)$

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

PAGE 1-A

$$\begin{array}{c} \circ \\ \text{Me-S-O} \\ \circ \\ \circ \\ \text{O-CH}_2\text{-CH}_2 \\ \end{array} \begin{array}{c} \text{CO}_2\text{H} \\ \text{CH}_2\text{-CH-S-CH}_2\text{-CH}_2 \\ \end{array}$$

PAGE 1-B

__ OH

CM 2

CRN 768-94-5 CMF C10 H17 N

RN 817209-96-4 CAPLUS

CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with α-[[2-(4hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]benze nepropanoic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 840494-28-2 CMF C26 H27 O7 S2

PAGE 1-A

$$\begin{array}{c} \circ \\ \text{Me-s-o} \\ \circ \\ \circ \\ \text{O} \\ \text{O-CH}_2\text{-CH}_2 \\ \end{array} \\ \begin{array}{c} \text{CO}_2\text{-} \\ \text{CH}_2\text{-CH-s-CH}_2\text{-CH}_2 \\ \end{array}$$

PAGE 1-B

__ OH

CM 2

CRN 62-49-7 CMF C5 H14 N O

 $Me_3+N-CH_2-CH_2-OH$

IT 549494-39-5P

RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of amine salts of [(phenoxyethyl)phenyl]propanoic acid derivative

useful for the treatment of lipid disorders)

RN 549494-39-5 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 549494-28-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation of amine salts of [(phenoxyethyl)phenyl]propanoic acid derivative

useful for the treatment of lipid disorders)

RN 549494-28-2 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

__ OH

REFERENCE COUNT:

3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2004:1154660 CAPLUS

DOCUMENT NUMBER:

142:93534

TITLE:

Substituted 3-phenylpropionic acid derivatives with

 $PPAR\alpha$ and $PPAR\delta$ modulatory activities,

useful as therapeutic agents for treatment of

dyslipidemia, and their preparation, pharmaceutical

compositions, and methods of use

INVENTOR(S):

Lindstedt-Alstermark, Eva-Lotte; Boije, Anna Maria

Persdotter; Holm, Patrik

PATENT ASSIGNEE(S):

Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE:

PCT Int. Appl., 52 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.					KIN	D	DATE			APPL	ICAT	ION :		DATE						
WO 2004113282					A1 20041229				WO 2	004-	 GB25		20040616							
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA.	CH.			
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD.			
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,			
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,			
		NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,			
		ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	ZW			
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	ΜZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,			
		AZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM,	ΑT,	ΒE,	BG,	CH,	CY,	CZ,	DE,	DK,			
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,			
		SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,			
		SN,	TD,	TG													•			
AU 2004249474									AU 2004-249474							0040	ZW, AM, DE, DK, RO, SE, MR, NE,			
CA 2529297									CA 2004-2529297						0040	616				
EP	1638927						0329	EP 2004-736926						20040616						
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,			
		ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR.	BG.	CZ.	EE.	HU.	PΤ.	SK	HP		

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BR 2004011536
                         Α
                                20060801
                                           BR 2004-11536
                                                                   20040616
    CN 1835917
                         Α
                               20060920
                                           CN 2004-80023273
                                                                   20040616
    JP 2006527747
                         Т
                               20061207
                                           JP 2006-516423
                                                                   20040616
    NO 2005006005
                         Α
                               20060224
                                           NO 2005-6005
                                                                   20051216
    US 2006199857
                         A1
                               20060907
                                           US 2005-561126
                                                                   20051216
PRIORITY APPLN. INFO.:
                                           GB 2003-14075
                                                                  20030618
                                           WO 2004-GB2554
                                                               W 20040616
```

OTHER SOURCE(S): MARPAT 142:93534

RN

CN

Substituted 3-phenylpropionic acid derivs. I are disclosed [R = H, OH or NH or their derivs.; R1 = alk(en/yn)yl, aryl, cyano, OH or SH or CO2H or their derivs.; R2 = H, alkyl, aryl, alkylaryl; R3, R4 = (independently) H, alkyl, aryl, alkylaryl; or R2R4 = pi bond; n = 1-6; m = 0 or 1; D's = H or wide variety of substituents; T = 0, S, or N(X) with some restrictions; X = alkyl or alkylaryl; with 2 complex provisos]. Also disclosed are (1) processes for preparing I, (2) their utility in treating clin. conditions including lipid disorders (dyslipidemias), whether or not associated with insulin resistance and other manifestations of the metabolic syndrome, (3) methods for their therapeutic use, and (4) pharmaceutical compns. containing them. I were tested in the assays described in WO 03/051821 (no data). I show superior potency in vitro, higher affinity, and/or higher in vivo efficacy. I also have a better selectivity profile, which is expected to improve in vivo safety. In addition, I may have improved DMPK (drug metabolism and pharmacokinetic) properties, for example improved metabolic stability in vitro or bioavailability. The compds. also have an improved solubility and/or a promising toxicol. profile. I may be combined with other therapeutic agents that are useful in the treatment of disorders associated with the development and progress of atherosclerosis such as hypertension, hyperlipidemias, dyslipidemias, diabetes and obesity. Twelve examples were prepared and/or claimed. For instance, compound II was prepared by: (1) thioetherification of 4-(PhCH2O)C6H4CH2CH2SH with ClCH(CO2Me)CH2C6H4(CH2CH2OH)-4 (40%); (2) Mitsunobu etherification of the product alc. with 4-benzoylphenol (83%); (3) debenzylation (78%); and (4) saponification of the ester with LiOH (49%). The EC50 of II for human PPARa was $0.78 \mu M$.

IT 817642-69-6P, 2-[[2-[4-(Dimethylamino)phenyl]ethyl]thio]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid 817642-71-0P, 2-[[2-(2-Fluorophenyl)ethyl]thio]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid 817642-72-1P, 2-[[2-(3-Methoxyphenyl)ethyl]thio]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid 817642-73-2P, 2-[[2-(4-Hydroxyphenyl)ethyl]sulfinyl]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid 817642-76-5P, 2-[[2-(4-Hydroxyphenyl)ethyl]sulfonyl]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid 817642-78-7P, 3-[4-[2-[2-Benzyl-4-[(methanesulfonyl)oxy]phenoxy]et hyl]phenyl]-2-[[2-(4-hydroxyphenyl)ethyl]sulfanyl]propionic acid 817642-79-8P, 2-[[2-(4-Tert-Butoxyphenyl)ethyl]sulfanyl]-3-[4-[2-[4-[(methanesulfonyl)oxy]phenoxy]ethyl]phenyl]propionic acid RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of substituted phenylpropionic acid derivs. as PPAR α and PPAR δ modulators for treatment of dyslipidemia) 817642-69-6 CAPLUS

Benzenepropanoic acid, α -[[2-[4-(dimethylamino)phenyl]ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ Me-s-O \\ O \\ O \\ O \\ O \\ CH_2-CH_2 \\ \end{array} \begin{array}{c} CO_2H \\ CH_2-CH-s-CH_2-CH_2 \\ \end{array}$$

PAGE 1-B

-NMe₂

RN 817642-71-0 CAPLUS

CN Benzenepropanoic acid, α -[[2-(2-fluorophenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

RN 817642-72-1 CAPLUS

CN Benzenepropanoic acid, α -[[2-(3-methoxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-B

[→] OMe

RN 817642-73-2 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]sulfinyl]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

__ OH

RN817642-76-5 CAPLUS

CNBenzenepropanoic acid, $\alpha - [[2 - (4 - hydroxyphenyl) ethyl] sulfonyl] - 4 - [2 - (4 - hydroxyphenyl) ethyl] sulfonyl]$ [4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

__ OH

RN817642-78-7 CAPLUS

Benzene
propanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-CN [(methylsulfonyl)oxy]-2-(phenylmethyl)phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

__ OH

817642-79-8 CAPLUS

RN Benzenepropanoic acid, α -[[2-[4-(1,1-dimethylethoxy)phenyl]ethyl]thi CN o]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2003:491173 CAPLUS

DOCUMENT NUMBER:

139:69050

TITLE:

Preparation of 3-phenyl-2-arylalkylthiopropionic acid

derivatives as selective agonists of PPAR- α

INVENTOR(S):

Alstermark Lindstedt, Eva-Lotte; Persdotter Boije,

Anna Maria; Holm, Patrik

PATENT ASSIGNEE(S):

Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE:

PCT Int. Appl., 47 pp.

DOCUMENT TYPE:

CODEN: PIXXD2 Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA'	PATENT NO.					KIND		DATE		APPLICATION NO.								
									WO 2002-GB5743									
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BE	BG,	BR.	BY.	BZ.	CA	CH.	CN	
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		GM,	HR,	HU,	ID,	IL	IN.	IS.	JP.	KE	, KG,	KP.	KR.	KZ.	T.C	', UE,	T.P	
		LS,	LT,	LU,	LV.	MA.	MD.	MG.	MK.	MN	, MW,	MX.	MZ.	NO.	NZ	OM	DH,	
		PL.	PT.	RO.	RU.	SC	SD.	SE.	SG.	SK	SL,	т.т	TM	ייו,	מידי	TTT	T11,	
		UA.	UG.	US.	UZ.	VC.	VN.	YU.	7A.	7.N	I, ZW	10,	,	-11,	110	.,,	14,	
	RW:	GH,	GM,	KE.	LS.	MW	MZ.	SD.	SL.	S7	, TZ,	UG.	7.M	7.W	ΔM	Ι Δ7.	BV	
		KG,	ĸz.	MD.	RU.	TJ.	TM.	AT.	BE.	BC	, CH,	CY	CZ.	DE.	את	r, re,	EC,	
		FI.	FR.	GB.	GR.	IE.	IT.	LU.	MC.	· NI	, PT,	SE,	ST.	SK	TP	BE	B.T	
		CF.	CG.	CI.	CM.	GA.	GN.	GO.	GW.	MT	. MR	NE.	SN.	תה	TC	., Dr,	, باب	
CA	2470066				A1 20030626					GW, ML, MR, NE, SN, CA 2002-2470066								
CA	2470		C 20070410															
AU	2002352426				A1	A1 20030630 AU						2002-352426				20021218		
EP	1458677				A1 20040922				EP 2002-788144				20021210					
	R:	AT,	BE,	CH,	DE,	DK.	ES.	FR.	GB.	GR	, IT,	T.T.	T.II.	NT.	SE	MC	DT.	
		IE,	SI,	LT,	LV.	FI	RO,	MK.	CY.	ΑI	, TR,	BG.	CZ.	EE.	SK		,	
BR	2002015090				Α	20041116				BR 2002-15090				20021218				
HU	2002015090 200402093				A2 20050228					HU 2004-2093					20021218			
JP	2005511785				T 20050428				JP 2003-552714					20021218				
JP	3810770				B2 20060816													
CN	1620430				Α		2005	0525		CN	2002-	8281	22			20021	218	
NZ	533365				A 20060526			0526	CN 2002-828122 NZ 2002-533365 ZA 2004-4585					20021218				
ZA	2004004585				A 20051026				ZA 2004-4585				20040609					
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PRIORITY	RIORITY APPLN. INFO.:									SE	2001-	4333			A	20011		
											2003-							
										WO	2002-	GB574	43	1	W	20021		
OTHER SC	THER SOURCE(S) ·				MADE	MAPDAT 139.69050			١									

OTHER SOURCE(S): MARPAT 139:69050

AB 4-(4-MeSO3C6H4OCH2CH2)C6H4CH2CH(CO2H)CH2CH2C6H4R-4 [I, R = Cl, F, OH] and optical isomers and racemates thereof were prepared for use in treating clin. conditions including lipid disorders (dyslipidemias) whether or not associated with insulin resistance. I have EC50 \leq 5 μ mol/L for PPAR- α and the ratio EC50 (PPAR- γ):EC50 (PPAR- α) > 25:1. Thus, I [R = Cl] was prepared from 4-(4-MeSO3C6H4OCH2CH2)C6H4CH2CH(CO2H)Cl

and 4-ClC6H4CH2CH2SH.

IT 549494-32-8P 549494-39-5P

RL: PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 3-phenyl-2-arylalkylthiopropionic acid derivs. as selective agonists of $\textsc{PPAR-}\alpha)$

RN 549494-32-8 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-chlorophenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (-)- (9CI) (CA INDEX NAME)

Rotation (-).

RN 549494-39-5 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 549494-27-1P 549494-28-2P 549494-29-3P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 3-phenyl-2-arylalkylthiopropionic acid derivs. as selective agonists of PPAR- α)

RN 549494-27-1 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-chlorophenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} \circ \\ \text{Me-s-o} \\ \circ \\ \circ \\ \text{O} \end{array}$$

PAGE 1-B

_ c1

RN 549494-28-2 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ Me-s-O \\ O \\ O \\ O \\ O \\ O-CH_2-CH_2 \\ \end{array} \\ \begin{array}{c} CO_2H \\ CH_2-CH-s-CH_2-CH_2 \\ \end{array}$$

PAGE 1-B

__ OH

RN 549494-29-3 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-fluorophenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} \circ \\ \text{Me-S-O} \\ \circ \\ \circ \\ \text{O} \\ \text{O-CH}_2\text{-CH}_2 \\ \end{array} \begin{array}{c} \text{CO}_2\text{H} \\ \text{CH}_2\text{-CH}_2\text{-CH}_2 \\ \text{CH}_2\text{-CH}_2 \\ \end{array}$$

PAGE 1-B

__ F

REFERENCE COUNT:

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ACCESSION NUMBER: 2003:491173 CAPLUS

DOCUMENT NUMBER:

139:69050

ENTRY DATE:

Entered STN: 27 Jun 2003

TITLE:

Preparation of 3-phenyl-2-arylalkylthiopropionic acid

derivatives as selective agonists of PPAR- α

INVENTOR(S): Alstermark Lindstedt, Eva-Lotte; Persdotter Boije, . Anna Maria; Holm, Patrik

PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE:

PCT Int. Appl., 47 pp.

CODEN: PIXXD2 DOCUMENT TYPE: Patent

LANGUAGE: INT. PATENT CLASSIF.:

MAIN:

C07C323-56

English

SECONDARY:

A61K031-192

CLASSIFICATION:

25-17 (Benzene, Its Derivatives, and Condensed

Benzenoid Compounds)

Section cross-reference(s): 1

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DATE APPLICATION NO. DATE PATENT NO. KIND ----_____ _____ ------20030626 WO 2002-GB5743 20021218 <--WO 2003051826 A1 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG CA 2470066 A1 20030626 CA 2002-2470066 20021218 C CA 2470066 20070410 AU 2002352426 A1 A1 AU 2002-352426 EP 2002-788144 20030630 20021218 EP 1458677 20040922 20021218 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK Α BR 2002015090 20041116 BR 2002-15090 20021218 HU 200402093

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SE 2001-4333 20050228 HU 2004-2093 20050428 JP 2003-552714 HU 200402093 20021218 20021218 20021218 20021218 20040609 20040610 NO 2004-300-US 2005-499042 20050320 JP 2006-77296 20060320 SE 2001-4333 A 20011219 JP 2003-552714 A3 20021218 US 2002-GB5743 W 20021218 20040716 PRIORITY APPLN. INFO.: PATENT CLASSIFICATION CODES: PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES -----______ WO 2003051826 ICM C07C323-56 ICS A61K031-192 IPCI C07C0323-56 [ICM, 7]; C07C0323-00 [ICM, 7, C*]; A61K0031-192 [ICS,7]; A61K0031-185 [ICS,7,C*] A61K0045-00 [I,C*]; A61K0045-00 [I,A]; A61K0031-185 IPCR [I,C*]; A61K0031-192 [I,A]; A61K0031-21 [I,C*]; A61K0031-255 [I,A]; A61K0031-366 [I,C*]; A61K0031-366 [I,A]; A61K0031-40 [I,C*]; A61K0031-40 [I,A]; A61P0003-00 [I,C*]; A61P0003-00 [I,A]; A61P0003-04 [I,A]; A61P0003-06 [I,A]; A61P0003-10 [I,A]; A61P0009-00 [I,C*]; A61P0009-10 [I,A]; A61P0009-12 [I,A]; C07C [I,S]; C07C0309-00 [I,C*]; C07C0309-66 [I,A]; C07C0319-00 [I,C*]; C07C0319-20 [I,A]; C07C0323-00 [I,C*]; C07C0323-56 [I,A]; C07D [I,S]; C07D0221-00 [I,C*]; C07D0221-18 [I,A]; C07K0014-435 [I,C*]; C07K0014-705 [I,A] **ECLA** C07C323/56 CA 2470066 A61K0031-192 [I,A]; A61K0031-185 [I,C*]; A61K0031-255 IPCI [I,A]; A61K0031-21 [I,C*]; A61K0031-366 [I,A]; A61K0031-40 [I,A]; A61K0045-00 [I,A]; A61P0003-04 [I,A]; A61P0003-06 [I,A]; A61P0003-10 [I,A]; A61P0003-00 [I,C*]; A61P0009-10 [I,A]; A61P0009-12

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                         4C206/ZA70; 4C206/ZC02; 4C206/ZC33; 4C206/ZC35;
                         4H006/AA01; 4H006/AA03; 4H006/AB20; 4H006/AB27;
                         4H006/TA04; 4H006/TB02; 4H006/TB40; 4H006/TB53;
                         4H006/TC32; 4H006/TC36
OTHER SOURCE(S):
                          MARPAT 139:69050
ABSTRACT:
4-(4-MeSO3C6H4OCH2CH2)C6H4CH2CH(CO2H)CH2CH2C6H4R-4 [I, R = Cl, F, OH] and
optical isomers and racemates thereof were prepared for use in treating clin.
conditions including lipid disorders (dyslipidemias) whether or not associated
with insulin resistance. I have EC50 \leq 5 \mumol/L for PPAR-\alpha and
the ratio EC50(PPAR-\gamma):EC50(PPAR-\alpha) > 25:1. Thus, I [R = Cl] was
prepared from 4-(4-MeSO3C6H4OCH2CH2)C6H4CH2CH(CO2H)Cl and 4-C1C6H4CH2CH2SH.
                   aralkylthiophenylpropanoic acid prepn peroxisome
SUPPL. TERM:
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proliferator activated receptor modulator

INDEX TERM: Dyslipidemia

ROLE: BSU (Biological study, unclassified); BIOL (Biological

study) (preparation of 3-phenyl-2-arylalkylthiopropionic acid derivs. as selective agonists of PPAR- α) INDEX TERM: Peroxisome proliferator-activated receptors ROLE: BSU (Biological study, unclassified); BIOL (Biological study) (α; preparation of 3-phenyl-2-arylalkylthiopropionic acid derivs. as selective agonists of PPAR- α) INDEX TERM: 549494-32-8P 549494-39-5P ROLE: PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of 3-phenyl-2-arylalkylthiopropionic acid derivs. as selective agonists of PPAR- α) INDEX TERM: 96-33-3, Methyl acrylate 103-16-2, 4-Benzyloxyphenol 104-10-9, 2-(4-Aminophenyl)ethanol 332-43-4, 1-(2-Chloroethyl)-4-fluorobenzene 507-09-5, Thioacetic acid, reactions 32327-70-1, 1-Chloro-4-(2-Chloroethyl) benzene 549494-36-2 ROLE: RCT (Reactant); RACT (Reactant or reagent) (preparation of 3-phenyl-2-arylalkylthiopropionic acid derivs. as selective agonists of PPAR- α) INDEX TERM: 455267-22-8P 549494-30-6P 549494-31-7P 549494-33-9P 549494-34-0P 549494-35-1P 549494-37-3P 549494-38-4P 549494-40-8P ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of 3-phenyl-2-arylalkylthiopropionic acid derivs. as selective agonists of PPAR- α) . INDEX TERM: 549494-27-1P 549494-28-2P 549494-29-3P ROLE: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of 3-phenyl-2-arylalkylthiopropionic acid derivs. as selective agonists of PPAR- α) REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD.

(1) Astra; WO 9962871 A 1999 CAPLUS(2) Astra; WO 9962872 A 1999 CAPLUS

REFERENCE(S):